Adv. Studies Theor. Phys., Vol. 8, 2014, no. 15, 653 - 654
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http://dx.doi.org/10.12988/astp.2014.4556

Self-Diffusion Coefficient of Liquid Rubidium

I. E. Furman

Ural Federal University, Mira str. 19, 620002, Ekaterinburg, Russia

Abstract

The self-diffusion coefficient of the liquid rubidium at *T*=312K is calculated in the square-well model within the random phase approximation. A good agreement with available experimental data is achieved.

Keywords: Square-well model, random phase approximation, self-diffusion coefficient, liquid metal

Earlier, the square-well (SW) model in the random phase approximation with the hard-sphere reference system had been successfully applied to study the self-diffusion coefficient, $D=(\beta\xi)^{-1}$ (where ξ is the friction coefficient, $\beta=(k_{\mathrm{B}}T)^{-1}$, k_{B} - Boltzmann constant, T - temperature), of liquid Na and K near their melting points [1, 2]. Here, this approach is used to calculate D of the liquid Rb at the same condition.

The Davis-Palyvos [3] approach is used for this aim:

$$\xi=\xi_{\mathrm{H}}+\xi_{\mathrm{S}}+\xi_{\mathrm{SH}} \quad , \tag{1}$$

where ξ_{H} and ξ_{S} are the contributions due to the hard and soft part of the pair interaction, respectively, ξ_{SH} - the cross-correlation term:

$$\xi_{\mathrm{H}}=\frac{8}{3}\rho\sigma^2 g(\sigma)(\pi M/\beta)^{1/2} \quad , \tag{2}$$

$$\xi_{\mathrm{S}}=-\frac{(\beta\pi M)^{1/2}}{12\pi^2}\int_0^\infty [S(q)-1]\phi(q)q^3\mathrm{d}q \quad , \tag{3}$$

$$\xi_{\mathrm{SH}}=-\frac{1}{3}\rho\, g(\sigma)(\beta M/\pi)^{1/2}\int_0^\infty [q\sigma\cos(q\sigma)-\sin(q\sigma)]\phi(q)\mathrm{d}q \quad , \tag{4}$$

where ρ is the mean atomic density (taken here from [4]), σ - hard-core dia-

meter, $g(r)$ - radial distribution function, M - atomic mass, $S(q)$ - structure factor, $\phi(q)$ - Fourier transform of the soft part of the pair potential. The SW model parameters for liquid Rb are defined by fitting the first peak of the structure factor with respect to the experimental one [5].

Calculated D in comparison with two experimental results is presented in Table 1.

Table 1. Self-diffusion coefficient of liquid Rb at T = 312 K.

	SW	Experiment [6]	Experiment [7]
$D{\cdot}10^{-9}$ (m^2/s)	3.15	2.68	2.22

It can be seen that the SW model gives slightly overstated value of D in comparison with experimental ones, similar to the cases of liquid Na [1] and K [2].

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Received: May 11, 2014